Russian Journal of Physical Chemistry A 2004 vol.78 N2, pages 238-243

The influence of intermolecular interactions on the internal dynamics of para-substituted 1,2-diphenylethanes

Kamalova D., Petrova S., Remizov A., Skochilov R., Chachkov D.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The IR absorption spectra and internal rotation of 1,2-di(para-XC 6H4)ethanes (X = H, Br, NO2) were studied in the crystalline and liquid phases and solutions at various temperatures. The thermodynamic parameters of conformational equilibria were determined. The concentrations of the conformers were found by factor analysis techniques. The trans and gauche conformers were studied by ab initio quantum-chemical calculations. The obtained differences of the Gibbs energies and entropies of the conformers were considered in terms of the reaction field model. The presence of the compensation effect in the thermodynamics of conformational transitions was substantiated.